

Philosophical Magazine Eirst Published in 1798

Physics of Condensed Matter

A Defects and Mechanical Properties

B Electronic Optical and Magnetic Properties



PHILOSOPHICAL MAGAZINE

Editor:

Professor E. A. Davis

Associate Editors:

Professor A. J. FORTY

Dr. P. M. HAZZLEDINE

Dr. M. J. GORINGE

Dr. S. R. ELLIOTT

Regional Editors:

Professor A. SEEGER (Stuttgart) Professor K. Morigaki (Tokyo)

Professor C. Domb (Bar-Ilan)

Dr. C. Schlenker (CNRS-Grenoble)

Consultant Editor:

Professor Sir Nevill Mott

Book Review Editor:

Dr. E. Marseglia

Subscription Information

Published monthly

Annual subscription 1984 £207 DM 966 US \$588

ISSN 0141 8610

Dollar rates apply to USA, Canada and Mexico. Deutschmark rates to FR Germany. Sterling rates apply to the UK and all other areas.

All subscriptions are payable in advance and all rates include postage. Journals are sent by air to the USA, Canada and Mexico, India and Australasia. Subscriptions are entered on an annual basis, i.e. from January to December, Payment may be made by sterling cheque, dollar cheque, international money order or National Giro, or by credit card (AMEX, VISA, Mastercard Access).

Orders originating in the following territories should be sent direct to the local distributors

USA, Canada and Mexico Japan India

Taylor & Francis Inc. 242 Cherry Street, Philadelphia, Pennsylvania 19106–1906. Kinokuniya Company Ltd. Odakyu West-Shinjuku Building. 47. I Hatsudai 1-ehome, Shibuya-ku, Tokyo 151. Universal Subscription Agency Pvt. Ltd. 11.7 H. 1. 294B Model Town, Pandu Nagar, Kanpur 208–025, Taylor & Francis Ltd. Rankine Road, Basingstoke, Hampshire RG24 0PR.

UK and all other territories

Air freight and mailing in the USA by Publications Expediting Inc., 200 Meacham Avenue, Elmont, New York 11003. Second class postage paid at Jamaica, New York 11431. US Postmaster: Send address changes to *Philosophical Magazine*, Publications Expediting Inc., 200 Meacham Avenue, Elmont, New York 11003.

Published by Taylor & Francis Ltd. 4 John Street, London WCIN 2ET, UK. Printed by Taylor & Francis (Printers) Ltd. Rankine Road, Basingstoke, Hampshire RG24 0PR. UK

Copyright © 1984 Taylor & Francis Ltd

All rights reserved. Authors are themselves responsible for obtaining permission to reproduce copyright material from other sources and are required to sign a form for agreement of the transfer of copyright. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form, or by any means, electronic, electrostatic, magnetic, mechanical, photocopying, recording or otherwise, without prior permission in writing from the copyright holder. 0141–8610-84-S3-00 (1984-Taylor & Francis Ltd.

Authorization to photocopy items for internal or personal use, or the internal or personal use of specific clients, is granted by Taylor & Francis Ltd for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service, provided that the base fee is paid directly to CCC, 21 Congress Street, Salem, Massachusetts 01970, USA. (For fee per article see copyright code above.) This consachusetts of the control of Fees for past articles are the same as those shown for current articles.

CONTENTS OF VOL. 49 Nos 1-6

NUMBER 1—JANUARY

PART A

	PAGE
Dielectric properties due to crystallographic shear planes in chromia-doped rutile (TiO ₂)	
By E. IGUCHI, K. OGINO, N. FURUHATA and R. J. D. TILLEY	1
Diffusion correlation and isotope effects in high-defect-content solids By G. E. Murch.	21
Solute drag on moving edge dislocations By R. Fuentes-Samaniego, R. Gasca-Neri and J. P. Hirth	31
Weak beam observation of dissociated dislocations in an Ll ₂ ordered alloy deformed at the temperature of strength anomaly By P. Veyssière, D. L. Guan and J. Rabier	45
Thermodynamic equilibrium in stressed systems. VI. Interfacial equations of	
By A. J. B. Spaull	55
Thermodynamic equilibrium in stressed systems. VII. Heats of adsorption By A. J. B. Spaull	63
Triple lines in polycrystalline aggregates as disclinations By W. Bollmann	73
Surface structure and energetics of multiply twinned particles By L. D. Marks	81
Elastic strains and the energy balance for multiply twinned particles By A. Howie and L. D. Marks	95
Pre-precipitation studies in an Al–Zn alloy by positron Doppler broadening measurements	
By S. Panchanadeeswaran, M. R. Plichta and J. G. Byrne	111
Temperature dependence of positron annihilation characteristics in Al-8.5 wt%Zn By S. Panchanadeeswaran and J. G. Byrne	139
An analysis of the unmixing kinetics of aluminium alloys in terms of nucleation and spinodal decomposition models By J. P. SIMON, P. GUYOT and A. GHILARDUCCI DE SALVA	151
The atomic structure of the NiSi ₂ -(001)Si interface By D. CHERNS, C. J. D. HETHERINGTON and C. J. HUMPHREYS	165

Letters Section:	PAGE
On the margin effect in section patterns obtained by plane-wave X-ray topography	L1
By K. Ishida, Y. Kobayashi and H. Katoh	LI
Fresnel effects at grain-boundary dislocations By C. B. BOOTHROYD and W. M. STOBBS	L5
PART B	
Electrical conductivity measurements on amorphous semiconductors of the system $(As_2Se)_{1-x}$: $(Tl_2Se_3)_x$	
By C. A. Majid	1
Photoluminescence et propriétés optiques d'alliages Si _x C _{1-x} amorphes préparés	
par depôt chimique en phase vapeur	
Par J. P. Gérault, R. Morancho et G. Constant	11
Monte Carlo simulation of the time dependence of geminate recombination	
By B. Ries, G. Schönherr, H. Bässler and M. Silver	27
by B. Kills, O. Scholalikk, H. Dasselk and M. Sievek	
Core structure and electronic bands of the 90° partial dislocation in silicon	
By K. W. Lodge, S. L. Altmann, A. Lapiccirella and N. Tomassini	41
Raman studies of non-stoichiometric amorphous GaSb films	62
By R. Carles, J. B. Renucci, A. Gheorghiu and ML. Theye	63
Bombardment with energetic hydrogen atoms during the sputter deposition of	
amorphous hydrogenated silicon	
By J. Tardy and R. Meaudre	73
Screening of ions in concentrated solutions	0.2
By M. Cutler	83
Electronic charge densities and the recursion method	
By R. Jones and M. W. Lewis	95
The thermal expansion of amorphous arsenic	
By M. A. Brown, I. J. Brown and A. R. Khan	101
Book reviews	107
Letters Section:	
On the analysis of space-charge-limited current-voltage characteristics and	
the density of states in amorphous silicon	
By J. W. Orton	L1
On the transport mechanism in chalcogenide glasses	
By H. Overhof and W. Beyer	L9
Disorder effects on deep trapping in amorphous semiconductors	
By R. A. Street	L15
	L13
Is there a phase transition to the re-entrant spin glass?	
By B. R. Coles	L21

NUMBER 2—FEBRUARY

PART A

Letters Section:	PAGE
EXAFS spectra for amorphous and crystalline Mg-Zn By M. Ito and T. Kawamura	L9
The effect of elastic anisotropy on contrast in the scanning acoustic microscope By M. G. Somekh, G. A. D. Briggs and C. Ilett	179
Role of α precipitates in flux pinning in a superconducting Ti–Nb–Ta–Zr quaternary alloy By K. Osamura, H. Tsunekawa, Y. Monju and T. Horiuchi	205
Determination of the duration of transient phenomena by frequency-domain analysis of acoustic emission	
By K. Takashima, Y. Higo and S. Nunomura	221
The propagation velocity of the martensitic transformation in 304 stainless steel By K. Takashima, Y. Higo and S. Nunomura	231
The strain distribution in anisotropic polycrystalline aggregates subjected to an	
external stress field By C. M. SAYERS	243
Solute and solvent diffusion in V–Zr alloys By D. D. Pruthi and R. P. Agarwala	263
The creep of nickel under pulsed electron irradiation By L. N. Bystrov, L. I. Ivanov and A. B. Tsepelev	273
Characterization of metal precipitates in magnesium oxide. Part I By J. Narayan, Y. Chen, R. M. Moon and R. W. Carpenter	287
A quasiharmonic calculation of perfect-crystal and intrinsic-defect properties of β-PbF ₂	
By P. W. M. JACOBS, V. C. SAHNI and C. S. VEMPATI	301
Self-diffusion of gallium and antimony in GaSb	
By D. Weiler and H. Mehrer	309
Burgers vector determination of dislocations in an elastically anisotropic crystal by high-order reflection imaging technique in a HVEM By H. SAKA	327
PART B	
Thermopower of dilute aluminium alloys and α-brass at elevated temperatures By A. M. Rosenfeld and R. S. Timsit	111
Total Compton intensity from amorphous Ca–Al By D. R. CHIPMAN and L. D. JENNINGS	127

Study of defect structure of calcium sulphide By R. Pandey and J. H. Harding	135
The Hall effect in vitreous 80V ₂ O ₅ –20P ₂ O ₅ By A. Vomvas and M. Roilos	143
Investigation of the decomposition kinetics of the alloy $Cu_{2\cdot 00}Mn_{1\cdot 00}Al_{1\cdot 00}$ by means of electrical resistance measurement By J. Sołtys, M. Stefaniak and J. Holender	151
A model for luminescent emission from surface states in MgO and CaO powders By W. W. DULEY	159
Relations entre la structure électronique et la facilité de glissement dans les métaux hexagonaux compacts Par B. Legrand	171
Electronic transitions of high probability corresponding to X-ray absorption discontinuities By S. KAWATA	185
Kinetics of distant-pair recombination. II. Tunnelling non-radiative recombination By D. J. DUNSTAN	191
Book reviews	215
NUMBER 3—MARCH	
PART A	
Letters Section:	
Growth steps on an ice crystal grown from the vapour By M. Ohtomo and G. Wakahama	L13
Application of TEM extended electron energy loss fine structure to the study of aluminium oxide films By A. J. BOURDILLON, S. M. El-Mashri and A. J. Forty	341
A brittle to ductile transition in ice under tension By E. M. Schulson, P. N. Lim and R. W. Lee	353
Resolution of atomic steps on dislocations in rutile By L. A. Bursill and M. G. Blanchin	365
Strain-ageing in silver chloride. II. The effect of temperature on the representa- tive curve	
By M. T. Sprackling and H. Shalitt	383

	PAGE
Direct measurements of dislocation charges in Ca ²⁺ -doped KCl by using large electric fields By T. KATAOKA, L. COLOMBO and J. C. M. LI	395
Dislocation charges in Ca ²⁺ -doped KCl. Effects of impurity concentration and	
temperature	
By T. Kataoka, L. Colombo and J. C. M. Li	409
Caging of an interstitial impurity in the vicinity of a collision cascade By V. V. Kirsanov and E. M. Kislitcina	425
Contrast of heavily decorated dislocations in optical birefringence micrographs By B. K. TANNER	435
Multiaxial creep laws based on dislocation glide By P. R. Schwab	445
	, ,,,
In situ TEM observation of dislocation motion in II–VI compounds By K. Suzuki, M. Ichihara, S. Takeuchi, K. Nakagawa, K. Maeda and H. Iwanaga	451
An electron diffraction study of ω -tricosenoic acid Langmuir–Blodgett films By I. R. Peterson and G. J. Russell.	463
PART B	
Letters Section:	
Time-dependent non-equilibrium exciton diffusion in an organic glass By R. Richert, B. Ries and H. Bässler	L25
Evidence of equilibrium native defect populations in amorphous chalcogenides from analyses of xerographic spectra By M. Abkowitz and J. M. Markovics	L31
Xerographic determination of electron drift mobility in a-Si:H	
By M. ABKOWITZ and R. C. ENCK	L37
The electrical conductivity and thermopower of films of amorphous tungstic oxide By C. B. Thomas and M. R. Goulding	219
Steady-state photoconductivity in amorphous semiconductors containing corre-	
By H. OKAMOTO, H. KIDA and Y. HAMAKAWA	231
Thermopower of sputtered amorphous Si(Ga) alloys By Le Xu, C. L. Foiles and D. K. Reinhard	249
Time-dependent geminate recombination in the presence of disorder in the energy	
of the hopping sites	

	PAGE
Anomalous temperature dependence of space-charge-limited currents and photoconductivity in amorphous silicon By E. Bhattacharya and K. L. Narasimhan	271
Effect of pressure and temperature on the O-H and O-D stretching, and translational vibrations in the Raman spectrum of ice clathrate By G. P. JOHARI and H. A. M. CHEW	281
Magnetic order and phase transformation in Ni ₂ MnGa By P. J. Webster, K. R. A. Ziebeck, S. L. Town and M. S. Peak	295
IVAP-originated two-level systems and tunnelling atoms in lone-pair amorphous semiconductors	311
By G. Russo and L. Ferrari Book reviews	321
NUMBER 4—APRIL	
PART A	
Letters Section:	
The observation of semicoherent and incoherent f.c.c./b.c.c. interfaces using electron diffraction By R. C. Ecob and B. Ralph	L19
The quasi-liquid film on ice. Evidence from, and implications for contact charging events By G. J. Turner and C. D. Stow	L25
Physical properties of oxides containing metal precipitates. Part II By J. Narayan and Y. Chen	475
Plastic compression of spheres By M. M. Chaudhri, I. M. Hutchings and P. L. Makin	493
A theoretical and experimental study of the plastic deformation of f.c.c. crystals in plane strain compression	505
By J. H. Driver, A. Skalli and M. Wintenberger	505
Dislocation structures of β -CuZn deformed in compression between 25 and 300°C By H. Saka and M. Kawase	525
Phase transformations in Fe-Ni Invar alloys By P. L. ROSSITER and P. J. LAWRENCE	535
Optimization of parameters for dynamic recoil mixing of gold films deposited on silicon	
By P. Argyrokastritis, D. S. Karpuzov, J. S. Colligon, A. E. Hill	517

Investigations by SIMS of the bulk impurity diffusion of Ge in Si By P. Dorner, W. Gust, B. Predel, U. Roll, A. Lodding and H. Odelius	557
Structure of the Σ=9, 11 symmetrical tilt grain boundaries in germanium. Electron microscopy observations By A-M. Papon, M. Petit and JJ. Bacmann	573
Rectangular disclination loops. I. A universal technique By A. N. Pertsev, A. E. Romanov and V. I. Vladimirov	591
Errata	611
PART B	
Letters Section:	
The L _{III} absorption edge of copper By M. H. Heinonen and J. A. Leiro	L43
Surface contributions to the two-layer structure in the plasma deposition of a-Si: H By E. Sacher, J. Klemberg-Sapieha, M. R. Wertheimer, H. P. Schreiber and R. Groleau	L47
Light-induced changes, adsorbate effects and surface photovoltage in a-Si: H By S. Kumar and S. C. Agarwal	L53
Theory of non-radiative transitions in molecules and solids By S. G. Christov	325
Theory of non-equilibrium diffusive transport in disordered materials By M. Grünewald, B. Pohlmann, B. Movaghar and D. Würtz	341
Vacuum-ultraviolet generation of luminescence and absorption centres in a-SiO ₂ By J. H. Stathis and M. A. Kastner	357
Electron-momentum distribution and charge-transfer study of vanadium silicides By B. K. Sharma, S. Manninen, T. Paakkari, M. W. Richardson and S. Rundqvist	363
Deep electron level calculations for dislocations in Si and Ge. Recursion approach exploiting the translation symmetry By H. Veth and H. Teichler	371
Charge density wave depinning in TaS ₃ By H. Salva, Z. Z. Wang, P. Monceau, J. Richard and M. Renard	385
Book reviews	427

NUMBER 5—MAY

PART A

Letters Section:	PAGE
Equivalence of Bain and Zener transformations By J. RIFKIN	L31
DLTS study of the influence of plastic deformation on deep levels in n-type CdTe By F. Gelsdorf and W. Schröter	L35
Electron-energy-loss analysis of α -Fe dendrites formed by primary crystallization of a Fe $_{81}B_{13\cdot 5}Si_{3\cdot 5}C_2$ glass By J. Rzepski, J. P. Chevalier, P. Trebbia and C. Colliex	L43
Anisotropic distribution of dislocation loops in HVEM-irradiated Zr By M. Griffiths, M. H. Loretto and R. E. Smallman	613
Computer simulation of phenomenological coefficients for atom transport in a	
random alloy By A. R. Allnatt and E. L. Allnatt	625
Scanning Auger microscopy study of lanthanum partitioning in sphene-based	
glass-ceramics By W. H. Hocking, P. J. Hayward, D. G. Watson and G. C. Allen	637
An X-ray photoelectron spectroscopic investigation of the oxidation of manganese By J. S. Foord, R. B. Jackman and G. C. Allen	657
Electron microscopy of copper oxidation By R. H. MILNE and A. HOWIE	665
Etude en dynamique moléculaire des défauts créés par irradiation dans la silice vitreuse Par N. V. Doan	683
Computer simulation of the correlation factors in vacancy-pair diffusion in mixed	
NaCl-type crystals By R. Lindström and RL. Lindström	689
Coherent bremsstrahlung from kilovolt electrons in zone axis orientations By G. M. Reese, J. C. H. Spence and N. Yamamoto	697
Isotope effect and correlated impurity diffusion jump processes of Sn and In in silver	
By HJ. Rockosch and C. Herzig	717
PART B Letters Section:	
On the measurement of densities of states in amorphous semiconductors By V. Halpern	L57

	PAGE
Optical properties of neutron-irradiation-induced defects in single-crystal tellurium near the fundamental energy gap By U. NAGEL and A. SCHULTE	431
	151
Polydisperse particle size analysis by pulsed electric birefringence By K. Parslow and B. R. Jennings	457
Quantitative analysis of the bond rearrangement process during solid phase epitaxy of amorphous silicon By T. Saito and I. Ohdomari	471
	17.1
One-electron density of states in chalcogenide glasses By P. NAGY	481
Electronic and optical properties of glow-discharge amorphous silicon-carbon alloys	
By J. Bullot, M. Gauthier, M. Schmidt, Y. Catherine and A. Zamouche	489
Electrical resistivity of liquid noble-metal alloys. Roles of pseudopotential	
refinements By S. M. M. RAHMAN	503
Thickness dependence of properties of P- and B-doped hydrogenated amorphous	
silicon. I. Dark conductivity and photoconductivity By S. HASEGAWA, S. SHIMIZU and Y. KURATA	511
Thickness dependences of properties of P- and B-doped hydrogenated amorphous silicon. II. ESR, hydrogen vibrational spectra and optical absorption By S. HASEGAWA, S. SHIMIZU and Y. KURATA	521
Crystal-field effect in the determination of the dipole force tensor in transition-	
metal based alloys By G. Moraitis, J. Khalifeh and C. Demangeat	533
Book reviews	537
NUMBER 6—JUNE	
PART A	
The peaking effect in the internal friction of metals	
By P. Feltham	727
Implications of (e, 2e) scattering for inelastic electron diffraction in crystals. I. Theoretical	72.5
By V. W. MASLEN and C. J. ROSSOUW	735
Implications of (e, 2e) scattering for inelastic electron diffraction in crystals. II. Application of the theory	
By C. J. Rossouw and V. M. Maslen	743

	PAGE
The detection of the change in the mean inner potential at dislocations in grain boundaries in NiO By M. RÜHLE and S. L. SASS	759
Atomic structure of [011] and [001] near-coincident tilt boundaries in	
germanium and silicon By C. d'Anterroches and A. Bourret	783
An X-ray diffraction study of faulting in single crystals of cubic ZnS grown from	
the vapour phase By M. T. Sebastian and P. Krishna	809
Properties of high-angle (001) twist grain boundaries in alkali-halide bicrystals.	
A theoretical investigation By D. Wolf	823
The effect of a grain boundary structural transformation on sliding in $\langle 10\overline{1}0 \rangle$ -tilt zinc bicrystals	
By T. Watanabe, SI. Kimura and S. Karashima	845
Anisotropy of Zener relaxation in Cu ₃ Au	
By F. Povolo and A. F. Armas	865
Subject index	873
Index of authors (with titles)	878
List of contents	iii
PART B	
Letters Section:	
The XPS valence band of chromium J. A. Leiro and E. E. Minni	L61
	LUI
Low-frequency hopping conductivity in amorphous semiconductors By S. Summerfield and P. N. Butcher	L65
Thermally stimulated currents in a-Si:H	
By D. S. Misra, A. Kumar and S. C. Agarwal	L69
The conductivity near a mobility edge	
By N. F. Mott	L75
Proodoning of outended V and all and the control of	
Broadening of extended X-ray absorption fine structure arising from the finite lifetime of the K hole	
By D. G. Stearns	541
Thermal dehydrogenation of polysilane	
By P. John, B. C. Cowie and I. M. Odeh	559

	PAGE
Studies of the frequency-dependent admittances of Schottky barriers formed on sputtered hydrogenated amorphous silicon By I. G. Gibb and A. R. Long	565
Time-dependent dissociation of a geminate electron-hole pair in crystalline lattices. A Monte Carlo study By B. Ries, G. Schönherr, H. Bässler and M. Silver	597
Cathodoluminescence and polarization studies from individual dislocations in diamond By N. Yamamoto, J. C. H. Spence and D. Fathy	609
Local density of states via the recursion and the equation-of-motion methods. A comparative study By S. K. Bose	631
Pressure and temperature dependence of the O-H and O-D stretching vibrations in the Raman spectrum of ice By G. P. JOHARI and H. A. M. CHEW	647
Book reviews.	661
Subject index	665
Index of authors (with titles)	670
List of contents	iii